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CALCULATION OF EXACT EIGENFUNCTIONS OF SPIN AND ANGULAR MOMENTUM USING THE PROJECTION OPERATOR METHOD

by

Aubey Rotenberg

August 15, 1961

Institute of Mathematical Sciences

NEW YORK UNIVERSITY
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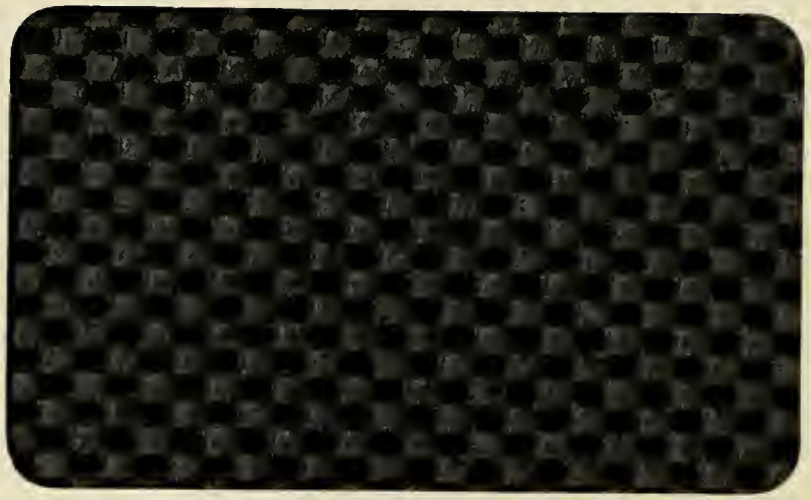

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ABSTRACT

The projection operator technique is used to generate electronic wave functions which are eigenfunctions of both spin and orbital angular momentum. All the functions which arise in the L-S coupling of any allowed system of electrons in a single s, p, d, or f shell are computed as well as some functions for a few electrons in the g-shell. In addition, functions arising in the coupling of electrons in different shells are obtained, and these eigenfunctions are of particular interest in configuration interaction studies of atomic structure. A few representative eigenfunctions are listed.

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CALCULATION OF EXACT EIGENFUNCTIONS OF SPIN AND ANGULAR MOMENTUM USING THE PROJECTION OPERATOR METHOD.

1. Introduction.

Since Löwdin[1] proposed the projection operator technique for constructing pure state angular momentum wave functions, the method has been applied to several calculations[2-6] only two of which have involved the use of electronic computers. Cooley[6] has written a program for the IBM-704 which computes spin angular momentum eigenfunctions under very general conditions. Abate and Fabri[5] have written a code for a small computer to calculate orbital angular momentum eigenfunctions, but the size of the computing machine used limited their work to a few electrons in a single shell, and even with these restrictions, the calculation of several states in the d-shell could not be completed because of overflow.

Described in this report is an extension of the work done by Abate and Fabri. Besides the obvious extensions which the use of a large scale computer permits, three important features have been incorporated in the code. In the first place, electrons are not restricted to be in a single shell and in fact can be distributed over as

many as eight different shells. Secondly, the functions are eigenfunctions of spin as well as of orbital angular momentum. And finally, in the case where there exist two or more independent terms of the same kind, the Gaussian elimination procedure is used to construct an orthogonal set of eigenfunctions. Condon and Shortley[7] have enumerated the expected terms in Russell-Saunders coupling for electrons in the p, d and f-shells. An auxiliary code has been written to extend this list to give the terms for two, three and four electrons in the g-shell as well as for electrons in two or more shells e.g. (sd), (pd), (pp) and (sdd). Some of these terms are listed in Table I.

2. The Angular Momentum Projection Operator.

The problem of resolving a wave function Ψ in components ϕ_{LM} having eigenvalues L and M has been considered by Löwdin.[1] Writing,

$$\Psi = \sum_L \sum_M c_{LM} \phi_{LM} \qquad (1)$$

where the summations are over all possible values of L and M. L is the orbital angular momentum and M is its component on the z-axis. Using the well-known eigenvalue relations for angular momentum, we have

$$\{\mathcal{L}^2 - L(L+1)\} \phi_{LM} = 0 \qquad (\mathcal{M} - M) \phi_{LM} = 0 \qquad (2)$$

where $\mathcal{L}$ and $\mathcal{M}$ are the operators corresponding to L and M respectively. Thus the eigenfunctions ϕ_{LM} are annihilated by both the operator $\{\mathcal{L}^2-L(L+1)\}$ and the operator $\{\mathcal{M}-M\}$. In this way it is possible to isolate a specific component $C_{LM}\phi_{LM}$ in (1) by annihilating all other components. This can be done[1] by means of the operators $\mathcal{O}_L$ and $\mathcal{O}_M$ defined as:

$$\mathcal{O}_L = \prod_{L'\neq L} \frac{\mathcal{L}^2-L'(L'+1)}{L(L+1)-L'(L'+1)} \tag{3}$$

$$\mathcal{O}_M = \prod_{M'\neq M} \frac{\mathcal{M}-M'}{M-M'} \tag{4}$$

where the denominators have been chosen for normalization purposes so that the operators give unity when working on the desired term.

Consider Φ to be a product (or, if antisymmetrization is effected, a sum of products) of one electron wave functions each having a principal quantum number, an orbital quantum number, ℓ; its z-component, m_ℓ; a spin quantum number, s $(= \frac{1}{2})$; its z-component, m_s $(= \pm \frac{1}{2})$. Then it is always possible to choose a function Φ having the desired eigenvalue M by requiring $\sum_i m_\ell = M$, where the summation is over all the electrons in the system. Thus the operator (4) need not be considered further. It should be emphasized, however, that this is purely a matter of convenience and that the

projection operator (4) could be used to generate eigenfunctions in a manner similar to that used in finding eigenfunctions of orbital angular momentum.

It is convenient in practice to consider the principal case viz. $M = L$, since if the eigenfunctions in this case are known, those for the other values of M are obtained easily be repeated use of the step-down operator $\mathcal{L}_-$. Introducing the identity $\mathcal{L}^2 = \mathcal{L}_- \mathcal{L}_+ + \mathcal{L}_z(\mathcal{L}_z+1)$ and making use of the fact that $\underline{\Phi}$ is now an eigenfunction having $M = L$ we can replace $\mathcal{L}_z$ by L and rewrite Eq. (3) in the form,

$$\mathcal{O}_{LL} = \prod_{L' \neq L} \frac{\mathcal{L}_- \mathcal{L}_+ + L(L+1) - L'(L'+1)}{L(L+1) - L'(L'+1)} \qquad (5)$$

where the double subscript makes explicit the fact that the principal case is meant. If we operate on a function $\underline{\Phi}$ assumed to have z-component equal to L, the terms in the product for which $L' < L$ will give zero. This is so because we have insured by our construction of $\underline{\Phi}$ that it has no components with angular momentum less than L, for the z-component of angular momentum must always be less than or equal to the total angular momentum. Thus, in the product only those values of $L' > L$ need be considered, the term $L' = L$ being explicitly excluded. Furthermore, there is a maximum possible value of L', say K, which can be ascertained from the given

assignment of L, total spin, the number of electrons and their individual shell assignments. By adding and subtracting a term in the denominator, Eq. (5) can be rewritten in the form

$$\mathcal{O}_{LL} = \prod_{L'=L+1}^{K} \left\{ \frac{\mathcal{L}_- - \mathcal{L}_+}{(L-L')(L+L'+1)} + 1 \right\} \tag{6}$$

3. The Computation Procedure.

In this section the computational procedure used to find exact eigenfunctions is described. Consider a system of n electrons distributed in H shells and coupled to have a total angular momentum L and multiplicity U = 2S+1, where S is the total spin. Defining μ as the number of α electrons (spin up) and ν as the number of β electrons (spin down), we have,

$$\begin{aligned} \mu &= \tfrac{1}{2}(n + U - 1) \\ \nu &= n - \mu \end{aligned} \tag{7}$$

Furthermore, the total number of components available for both α and β electrons is

$$P = \sum_{i=1}^{H} (2\ell_i + 1) \tag{8}$$

where ℓ_i is the orbital angular momentum of the electrons in the i^{th} shell.

These P components may be represented in binary notation by a string of P bits (a bit is defined as a "1" or a "0") such that an occupied orbital is represented by a "1" and an unoccupied orbital by a "0". We think of each bit position as representing a one electron wave function with a principal quantum number, ℓ, m_ℓ, s and m_s. For convenience, the bit position represents a specific ℓ and m_ℓ (as well as the principal quantum number) but the α and β electrons ($m_s = \pm 1/2$) are represented by separate machine words hereinafter referred to as patterns. Thus the bit positions in each pattern represent the quantum numbers ℓ_1, ℓ_1-1, ... $-\ell_1$+1, $-\ell_1$ for the values of the components for electrons in the first (i.e. $\ell = \ell_1$) shell; then ℓ_2, ℓ_2-1, ... $-\ell_2$ for the second shell and so on. μ electrons can be distributed in the P bit positions in $\binom{P}{\mu}$ ways, each giving a pattern consisting of μ "1"s and (P-μ) "0"s. Similarly ν electrons can be distributed in the P positions in $\binom{P}{\nu}$ ways. Since each bit represents an assigned component m, each pattern has associated with it a total z-component obtained by summing the values of m corresponding to those positions where the pattern has a "1". All possible pairs of patterns, one from the α set and one from the β set are examined and those pairs having both the assigned number of electrons in every shell and a total projection equal to the total angular

momentum L (for the principal case M = L) provide a basic set of N functions, denoted by $\underline{\Psi}_Q$. Operation by the projection operator (6) on any member of the set gives a function $\underline{\Phi}$ which is a linear combination of the members of the set. $\underline{\Phi}$ is thus an eigenfunction of $\mathcal{L}$ by the fundamental property of the projection operator, and an eigenfunction of $\mathcal{M}$ since each component of $\underline{\Phi}$ is an eigenfunction of $\mathcal{M}$ by construction. Furthermore the division into α and β patterns means that $\underline{\Phi}$ is constructed to be an eigenfunction of the z-component of spin.

So far we have not specified the relationship of a pattern to a wave function, although it has been made clear that a "1" in a bit position does represent an electron with a complete set of quantum numbers. From now on the pair of patterns making up an element $\underline{\Psi}_Q$ of the basic set is to be considered as the Slater determinant[3] constructed from the one electron wave functions which are in turn specified by "1"s in the patterns. The antisymmetrization implied here is nowhere carried out explicitly.

The projection operator (6) involves only one non-arithmetic operation, $\mathcal{L}_- \mathcal{L}_+$. Instead of expanding this operator in terms of its one electron components it is simpler to perform the operation on each basic function.

It is shown in the appendix, where some details of the computational method are outlined, that $\mathcal{L}_- \mathcal{L}_+$ can be decomposed into elements $(\mathcal{L}_-\mathcal{L}_+)_{QR}$ which connect just the Q^{th} and R^{th} elements of the basic set, such that

$$(\mathcal{L}_-\mathcal{L}_+)\,\Psi_Q = \sum_{R=1}^{N} (\mathcal{L}_-\mathcal{L}_+)_{QR}\,\Psi_R \,. \qquad (9)$$

Thus the operation $\mathcal{L}_-\mathcal{L}_+$ is equivalent to the matrix multiplication indicated. In general we operate on a linear combination of the basic set so that for one term in (6) we have,

$$\left\{\frac{\mathcal{L}_-\mathcal{L}_+}{(L-L')(L+L'+1)}+1\right\}\left[\sum_{Q=1}^{N} C_Q\,\Psi_Q\right] = \sum_{R=1}^{N}\sum_{Q=1}^{N} C_R\left[\frac{(\mathcal{L}_-\mathcal{L}_+)_{QR}}{(L-L')(L+L'+1)}+1\right]\Psi_R$$

$$= \sum_{R=1}^{N} C'_R\,\Psi_R \qquad (10)$$

where C_Q and C'_R are numerical factors, the latter being defined by the second part of Eq. (10). For the next value of L', the primed factors become the unprimed ones and at the end the latter give the linear combination specifying the desired eigenfunction.

The matrix elements $(\mathcal{L}_-\mathcal{L}_+)_{QR}$ have the form $a\sqrt{b}$ where a and b are integers (see Appendix). Since the denominator of the operator in (6) consists only of integers, all the numbers that must be dealt with are of the form $a\sqrt{b}/c$. Numbers of this type must be added and multiplied. In these calculations it is important to

preserve this representation in terms of integers since the round-off, introduced by approximating the surds and fractions would destroy the orthogonality of the wave functions rendering the approximate wave functions so obtained useless for many applications. The surds are easily handled since in all additions, the surds in both augend and addend are the same. It is only necessary to extract square factors from the surd after multiplication and this is done by examining the surd term b for factors $4, 4^2, \ldots, 9, 9^2, \ldots, 25$, etc., the process ending when the next square factor to be tried is larger than b. In order to prevent overflow, common factors must be removed from numerator and denominator after every arithmetic operation. This can be done by using the Euclidean algorithm to express the fraction as a continued fraction from which the normal form is obtained directly. In performing integer arithmetic of this kind it is good practice to extract common factors from both the numerators and the denominators before the multiplication (or addition) as this greatly reduces the danger of overflow.

The procedure described so far does not give spin eigenfunctions. Spin eigenfunctions could be generated by operating with a spin projection operator $\mathcal{O}_{SS}$ defined analogously to (3) where the second subscript indicates that $S_z = S$. Instead, an explicit formula

for the $\mathcal{O}_{SS}$ projection of a single Slater determinant[4] is used. For the Slater determinant built up from the μ orbitals having α spin and the ν orbitals having β spin we introduce the notation $[a^{\mu}|b^{\nu}]$ where a and b are abbreviations for the various ℓ and m values. For the sum of $\binom{\mu}{p} \times \binom{\nu}{p}$ determinants obtained from $[a^{\mu}|b^{\nu}]$ by interchanging p orbitals from the a group in order in all possible ways with p orbitals of the b group in order we introduce the notation $[a^{\mu-p}b^{p}|a^{p}b^{\nu-p}]$. Then the explicit formula[4] is

$$\mathcal{O}_{SS}\,[a^{\mu}|b^{\nu}] = \frac{2S+1}{\mu+1} \sum_{p=0}^{\nu} [a^{\mu-p}b^{p}|a^{p}b^{\nu-p}] \,. \qquad (11)$$

To get a spin eigenfunction one member of the basic set Ψ_Q is chosen. Operating with $\mathcal{O}_{SS}$ as given by (11) gives a linear combination of the basic set which is used as a starting function for (6). It is clear that the determinants obtained by the interchanges indicated on the right side of (11) are always members of the basic set. To minimize the number of interchanges needed, one may start with a basic function having as many doubly occuplied orbitals as is possible, consistent with the assignment of orbital angular momentum and multiplicity.

Where there are D $(D > 1)$ independent eigenfunctions with the same L and U, it is necessary to generate D separate functions. The starting functions

are chosen to be spin eigenfunctions, as described above, different starting functions being obtained by operating in (11) on a different member of the basic set. It is possible that the first D functions generated will not be linearly independent and in this case further functions are generated until a linearly independent set is obtained. Linear independence is established when the set of eigenfunctions is orthogonalized by the Gaussian elimination procedure without transforming any eigenfunction to zero. If one is transformed to zero this function is linearly dependent upon the others and is removed from the set of eigenfunctions and another one generated in its place. For the most part, it has been found that the first D functions generated do form an independent set. Integer arithmetic should be used in the Gaussian eliminations not only for the reasons given above, but also because otherwise it would be difficult to give an adequate criterion for zero to establish linear dependence of an eigenfunction.

4. Results and Applications.

A program has been written for the IBM-704 to generate spin and angular momentum eigenfunctions for electrons in several different shells. While the description given above, as well as the code itself,

refer to Russell-Saunders coupling only, the projection operator method applies equally well to j-j coupling and the code could be adapted to compute the eigenfunctions in j-j coupling.

All the results given by Abate and Fabri[5] for the d-shell have been duplicated but our functions are, of course, spin eigenfunctions in all cases whereas theirs are not. In addition, those few cases where their calculations failed due to overflow have now been computed. For the f-shell, they obtained most of the angular momentum eigenfunctions for f^3 and f^4; the IBM-704 code is able to compute all the eigenfunctions of spin and angular momentum for any number of electrons in a single f-shell in L-S coupling. We have obtained also some of the eigenfunctions for a few electrons in the g-shell, as well as several eigenfunctions for cases where electrons are distributed over two or more shells.

Because the tables of these eigenfunctions are lengthy, only a few representative functions are listed. In Table II, the electronic configuration and the spectroscopic designation of the term are given in the first column in the notation of Condon and Shortley.[7] The numeral under the term designation shows the number of terms of the kind, D, occurring in the configuration. In the second column the set of basic patterns Ψ_R is

listed. The α and β electrons are separated by a vertical bar. Electrons in different shells are separated by a comma, the shells being listed in the order given in the first column. A dash indicates that the pattern has no electrons in a shell. Thus ℓ, s and m_s are designated by position and only m_ℓ is listed explicitly. To conserve space a negative sign is indicated by a bar above the number. The third, and other columns if needed, list the coefficients C_R of the pattern given in the second column. An asterisk indicates which pattern was used to start with. Thus in terms of our notation

$$\mathcal{O}_{SS}\mathcal{O}_{LL}\Psi_Q = \sum_R C_R \Psi_R \quad . \tag{12}$$

The Q^{th} pattern is the starred one and the Ψ_R and C_R are listed in the second and third (and other) columns respectively. The result of performing the Gaussian elimination is not included in Table II.

Some of the examples have been taken from Condon and Shortley[7] (p. 217) where the concept of parentage is introduced. For the ^3H term arising from p^2d^2 the parentage given for the two terms is $p^2(^1D)d^2(^3F)$ and $p^2(^3P)d^2(^1G)$ and it is clear by inspection of the eigenvectors written in Table II that they correspond to these two cases respectively. On the other hand for the ^2F term arising from sdd, the parentages given are $sd(^1D)d$ and $sd(^3D)d$

and in this case it is easily seen that the eigenvectors given are linear combinations of these two terms. Thus in general the projection operator method of computing eigenfunctions does not preserve the parentage concept. While this may be of some disadvantage in some cases, the fact is that the concept itself is of somewhat limited usefulness; for example, where a group contains three or more equivalent d or f electrons, we cannot distinguish between the terms occurring more than once in this group except by giving the actual eigenfunctions.[7] Furthermore, in any calculation one set of eigenfunctions is as good as any equivalent set and will give the same observables.

The method of calculation described here makes explicit use of the binary character of the IBM-704, both for the representation of the Slater determinants and for various Boolean operations that are performed on them. It is certainly not necessary to use the binary notation to represent the patterns and in fact a decimal representation is given in Table II. However, the operations which are performed on the patterns do depend very intimately upon their binary nature and anyone who would want, for example, to code the projection operator technique for a decimal machine would of necessity be obliged to write a larger and more complicated code than the one described. Readers who are experienced coders for the IBM-704 will realize

that much of the coding for this problem must be done in direct machine code and that an automatic coding system such as FORTRAN is not flexible enough to generate the patterns needed and to operate on them.

This calculation was undertaken to determine the feasibility of computing spin and angular momentum eigenfunctions using the projection operator method. Dozens of such eigenfunctions have now been obtained. The time taken to get one eigenfunction using the IBM-704 code depends greatly upon the particular term involved and ranges up to about five minutes for terms such as the ^2P arising from a group of seven f electrons which has 114 basic patterns.

Work is now in progress to use these eigenfunctions in configuration interaction studies of atomic structure.

Appendix

Since $\mathcal{L}_{\pm}$ is an abbreviation for $(\ell_{1\pm} + \ell_{2\pm} + \ell_{3\pm} + \ldots)$ where the numerical subscripts refer to the electrons and ℓ_{i+} and ℓ_{i-} are the one electron step up and step down operators, we can write

$$\mathcal{L}_{-}\,\mathcal{L}_{+} = \sum_{i=1}^{n} \sum_{j=1}^{n} \ell_{i-}\,\ell_{j+} \tag{13}$$

Furthermore,

$$(\ell_{i-}\,\ell_{j+})\,\Psi_{Q} = a_{QR}\,\Psi_{R} \tag{14}$$

that is, each term $\ell_{i-}\,\ell_{j+}$ operating on a pattern Ψ_{Q} will give either another pattern in the set Ψ_{Q} multiplied by a factor a_{QR} or else zero. To get a_{QR} we recall that

$$\ell_{\pm}\,\phi_{m} = \sqrt{(\ell \mp m)(\ell \pm m + 1)}\;\phi_{\ell, m\pm 1} \tag{15}$$

where $\phi_{\ell m}$ is a normalized one electron wave function, so that a_{QR} is a product of two terms, each one of which is of the form of the factor on the right side of Eq. (15). It is clear from Eq. (15) that a_{QR} will automatically be zero if ℓ_{+} operates on $\phi_{\ell\ell}$ or ℓ_{-} on $\phi_{\ell_1 -\ell}$. There is another situation where the operation will give zero, namely, when ℓ_{+} (or ℓ_{-}) will try to step up (down) an electron into an orbital which is already occupied, since this would violate the Pauli exclusion principle.

In Eq. (14) it is important to notice that there is only one term on the right-hand side. Since two specified, i.e. i and j, electrons are altered by the operation such that one gains and the other loses one unit of z-component of angular momentum, the net sum of z-component remains the same so that the new pattern is a member of the basic set. Furthermore, no other $\ell_{i-}\ell_{j+}$ will connect Ψ_Q and Ψ_R, since these patterns differ only in the specified electrons. Thus, instead of summing over the electrons as in Eqs. (13) and (14) we can sum over the patterns and represent the operator $\mathcal{L}_-\mathcal{L}_+$ by a matrix with elements $(\mathcal{L}_-\mathcal{L}_+)_{QR}$. For $Q \neq R$, $(\mathcal{L}_-\mathcal{L}_+)_{QR} = a_{QR}$. If $i = j$ in Eq. (14), a single electron is first stepped up and then down, so $i = j$ implies $Q = R$. Subject to the restriction that neither of the factors ever gives zero, there may be several electrons which can contribute to the diagonal element and we can write

$$\sum_i (\ell_{i-}\ell_{j+})\Psi_Q = \sum_i a_{QQi}\Psi_Q = (\mathcal{L}_-\mathcal{L}_+)_{QQ}\Psi_Q \qquad (15)$$

where a_{QQi} is the contribution due to the i^{th} electron.

The formulation in terms of patterns, instead of electrons is purely for computational convenience. For the same reason, the bits within each shell are arranged in decreasing size of the value of m, the projection of

angular momentum. As an example consider three electrons in a d-shell with m = 2, 1, and -2. The bit pattern (11001) represents the Slater determinant for this case. We have already noted that the step up (down) operator changes the z-component by exactly one unit. Thus there will be non-zero contributions to the matrix $(\mathcal{L}_-\mathcal{L}_+)_{QR}$ only in cases where the patterns Ψ_Q and Ψ_R differ by one unit (one bit position) in exactly two positions and are the same elsewhere. This can be done by forming, in Boolean notation,

$$\chi_{QR} = \bar{\Psi}_Q \cap \Psi_R \tag{16}$$

and counting the number of "1" bits in χ_{QR}. Only if this number is exactly two will the matrix element be non-zero. Next it is necessary to check that the pairs of different bits are in adjacent positions. By forming χ_{RQ} and checking that the one bits in χ_{QR} and χ_{RQ} are adjacent in pairs the existence of a non-zero $(\mathcal{L}_-\mathcal{L}_+)_{QR}$ is finally established.

This procedure can be clarified by an example. Consider the ^4P state arising from three d-electrons in a single shell. There are just two basic functions, viz. Ψ_1 = (11001) and Ψ_2 = (10110). [All are α-electrons, there are no β-electrons in this case.] Then χ_{12} = (00110) and χ_{21} = (01001) and it is at once

clear that both pairs of bits are adjacent. This example makes evident, too, the effect of the $\ell_- \ell_+$ operation. In the machine the test for adjacency is made by appropriate shifts and comparisons. The step down factors corresponding to each bit position are stored and the step up factors are obtained directly from the step down factor for the next highest projection. Where there are two or more shells, this procedure might indicate that there exists a non-zero matrix element involving a transition between shells, but the step down factor for the projection $m = -\ell$ is zero. For the diagonal terms, each pattern is examined to see where there is a zero bit to the left of a one bit and each time this occurs, there is a contribution to the matrix element which is just the square of the step up factor associated with the one bit.

The elements of the $(\mathcal{L}_- \mathcal{L}_+)_{RS}$ matrix are calculated once and for all and stored in the machine for use in computing the desired eigenfunction. Only those elements on and above the main diagonal need be computed since $(\mathcal{L}_- \mathcal{L}_+)_{QR} = (\mathcal{L}_- \mathcal{L}_+)_{RQ}$.

Table I. Russell-Saunders Terms for Several Configurations

The numerals under the term designation show the number of terms of the kind occurring in the configuration.

Configuration	Terms			
g , g^{17}	^2G			
g^2, g^{16}	^1SDGIL	^3PFHK		
g^3, g^{15}	$^2P_{2}D_{2}F_{3}G_{3}H_{2}I_{2}K_{2}LMNO$	$^4P_{2}FGHIKM$		
g^4, g^{14}	$^1S_{3}D_{5}F_{2}G_{6}H_{3}I_{6}K_{3}LMNO_{5}Q_{2}T$	$^3P_{4}D_{3}F_{6}G_{5}H_{7}I_{5}K_{6}LMNO_{4}Q_{2}R$	$^5S_{2}D_{2}F_{2}G_{2}HIKLN$	
sd, sd^9	^1D	^3D		
sd^2, sd^8	^2SPDFG	^4PF		
sd^3, sd^7	$^1P_{2}DFGH$	$^3P_{2}DFGH_{2}$	^5PF	
sd^4, sd^6	$^2S_{2}PD_{2}FG_{3}HI_{3}$	$^4P_{2}DFGH_{2}$	^6D	
sd^5	$^1S_{3}PDFG_{2}HI$	$^3S_{2}PDFG_{4}HI_{3}$	^5SPDFG	^7S
pp	^1SPD	^3SPD		
pp^2	$^2S_{3}PDF_{2}$	^4SPD		
pp^3	$^1SPDF_{2}$	$^3S_{3}PDF_{2}$	^5P	
p^2p^2	$^1S_{3}PDFG_{4}$	$^3SPDF_{5}$	^5SPD	
p^2p^3	$^2S_{2}PDFG_{6}$	$^4SPDF_{2}$	^6P	

Table II. Some Representative Eigenfunctions

Config.	Term	Ψ	Eigenfunctions
f^6	^3L	$(3\bar{1}0\bar{1}\mid 32)$	$-47/171$ $\quad 4\sqrt{2}/57$ $\quad 2\sqrt{2}/57$
	3	$(3\bar{2}0\bar{2}\mid 32)$	$*\ 58/171$ $\quad -11\sqrt{2}/57$ $\quad 4\sqrt{2}/57$
		$(3\bar{2}0\bar{1}\mid 31)$	$-11/171$ $\quad 7\sqrt{2}/57$ $\quad -2\sqrt{2}/19$
		$(3\bar{2}1\bar{3}\mid 32)$	$-11\sqrt{2}/57$ $\quad *\ 14/19$ $\quad 2/57$
		$(3\bar{2}1\bar{2}\mid 31)$	$-5\sqrt{30}/171$ $\quad -4\sqrt{15}/57$ $\quad -2\sqrt{15}/57$
		$(3\bar{2}1\bar{1}\mid 21)$	$4\sqrt{2}/57$ $\quad 2/57$ $\quad *\ 20/57$
		$(3\bar{2}1\bar{1}\mid 30)$	$8/57$ $\quad 2\sqrt{2}/57$ $\quad \sqrt{2}/57$
		$(3\bar{2}10\mid 20)$	$-4\sqrt{2}/57$ $\quad -2/57$ $\quad -20/57$
		$(3\bar{2}10\mid 3\bar{1})$	$-4/57$ $\quad -\sqrt{2}/57$ $\quad 3\sqrt{2}/19$
f^7	^4L	$(321\bar{1}\bar{2}\mid 32)$	$*\ 29/57$ $\quad -14\sqrt{2}/57$ $\quad 5\sqrt{2}/57$
	3	$(3210\bar{3}\mid 32)$	$-14\sqrt{2}/57$ $\quad *\ 43/57$ $\quad 5/57$
		$(3210\bar{2}\mid 31)$	$-\sqrt{30}/19$ $\quad -\sqrt{15}/19$ $\quad -\sqrt{15}/19$
		$(3210\bar{1}\mid 21)$	$5\sqrt{2}/57$ $\quad 5/57$ $\quad *\ 43/57$
		$(3210\bar{1}\mid 30)$	$10/57$ $\quad 5\sqrt{2}/57$ $\quad -14\sqrt{2}/57$
f^5	^4K	$(320\bar{1}\mid 3)$	$*\ 35/68$ $\quad -11\sqrt{30}/136$
	2	$(321\bar{2}\mid 3)$	$-11\sqrt{30}/136$ $\quad *\ 81/136$
		$(321\bar{1}\mid 2)$	$-5\sqrt{2}/136$ $\quad -5\sqrt{15}/136$
		$(3210\mid 1)$	$3\sqrt{15}/68$ $\quad 15\sqrt{2}/136$
f^5	^4I	$(310\bar{1}\mid 3)$	$*\ 1/2$ $\quad -2/7$ $\quad 3\sqrt{2}/28$
	3	$(320\bar{2}\mid 3)$	$-2/7$ $\quad *\ 2/7$ $\quad -3\sqrt{2}/14$
		$(320\bar{1}\mid 2)$	$-\sqrt{15}/14$ $\quad 0$ $\quad \sqrt{30}/28$
		$(321\bar{3}\mid 3)$	$3\sqrt{2}/28$ $\quad -3\sqrt{2}/14$ $\quad *\ 19/28$
		$(321\bar{2}\mid 2)$	$5\sqrt{2}/28$ $\quad -\sqrt{2}/14$ $\quad -1/4$
		$(321\bar{1}\mid 1)$	$\sqrt{2}/28$ $\quad \sqrt{2}/14$ $\quad 1/28$
		$(3210\mid 0)$	$-\sqrt{2}/28$ $\quad -\sqrt{2}/14$ $\quad -1/28$
g^3	^4F	$(210\mid -)$	$*\ 761/2574$ $\quad 113\sqrt{7}/1287$
	2	$(31\bar{1}\mid -)$	$-761\sqrt{70}/25740$ $\quad -791\sqrt{10}/12870$
		$(32\bar{2}\mid -)$	$761\sqrt{70}/25740$ $\quad 791\sqrt{10}/12870$
		$(40\bar{1}\mid -)$	$113\sqrt{7}/1287$ $\quad *\ 448/1287$
		$(41\bar{2}\mid -)$	$-41\sqrt{70}/4290$ $\quad -161\sqrt{10}/2145$
		$(42\bar{3}\mid -)$	$-196\sqrt{10}/6435$ $\quad 94\sqrt{70}/6435$
		$(43\bar{4}\mid -)$	$98\sqrt{70}/6435$ $\quad -329\sqrt{10}/6435$
pd^2	^2F	$(-,20\mid 1,-)$	0 $\quad -\sqrt{3}/12$ $\quad 0$
	3	$(-,21\mid 0,-)$	0 $\quad 1/4$ $\quad 0$
		$(\bar{1},2\mid -,2)$	$*\ 7/9$ $\quad -7\sqrt{2}/36$ $\quad 1/9$
		$(0,1\mid -,2)$	$-7\sqrt{2}/36$ $\quad *\ 2/9$ $\quad -\sqrt{2}/36$
		$(0,2\mid -,1)$	$-7\sqrt{2}/36$ $\quad -1/36$ $\quad -\sqrt{2}/36$
		$(1,0\mid -,2)$	$\sqrt{6}/36$ $\quad -\sqrt{3}/18$ $\quad -5\sqrt{6}/36$
		$(1,1\mid -,1)$	$1/9$ $\quad -\sqrt{2}/36$ $\quad 4/9$
		$(1,2\mid -,0)$	$\sqrt{6}/36$ $\quad -\sqrt{3}/36$ $\quad -5\sqrt{6}/36$
p^2d^2	^3H	$(1,21\mid 1,-)$	$*\ 1$ $\quad 0$
	2	$(10,2\mid -,2)$	0 $\quad *\ 1$
sdd	^2F	$(-,1,2\mid 0,-,-)$	$*\ 1/3$ $\quad -1/6$
	2	$(-,2,1\mid 0,-,-)$	$-1/3$ $\quad 1/6$
		$(0,-,1\mid -,2-)$	$-1/6$ $\quad *\ 1/3$
		$(0,-,2\mid -,1,-)$	$1/6$ $\quad -1/3$
		$(0,1,-\mid -,-,2)$	$-1/6$ $\quad -1/6$
		$(0,2,-\mid -,-,1)$	$1/6$ $\quad 1/6$

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